

Probing the dynamics of proteins by MD simulations v.s. neutron scattering experiments

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Abstract

Detailed understanding of the function of several proteines requires the knowledge of their structure, energetics and dynamics at the atomic level. To probe the latter, Inelastic neutron scattering has emerged as a powerfull tool allowing the time-resolved study of motions taking place in the protein on the pico- to nanosecond time scale. Recently it has become possible to overcome the experimental limitations to investigate protein motions in environments ranging from low hydration powders to proteins in solution. We will show that combining such experiments to molecular dynamics simulations is necessary if one seeks to extract valuable informations about protein dynamics even in the case of simple systems.